

Quality standards for coconut oil and coco chemicals

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Introduction

Coconut oil is primarily used for edible purpose and as a hair oil. It is an important source of intermediates like fatty acids, glycerol and fatty alcohols, which are used for the manufacture of wide range of chemicals such as surfactants, emulsifiers, foam boosters etc. These intermediates are used in the formulation of several finished products like soaps, detergents and shampoos.

Coconut is one of the ten most useful trees in the world, providing food for millions of people, especially in the tropics. Regardless of its origin, the coconut has spread across much of the tropics and coastal areas. The fruit is light (approx 1kg) and buoyant and presumably spread significant distances by marine currents. India is one of the leading producers of coconut in the world.

Coconut oil is commonly referred to as lauric oil. The raw oil is obtained simply through mechanical pressing of dried copra without further treatment apart from filtration. The raw oil is preferred as it retains the compounds that provide its distinctive taste and odour. For marketing purposes, raw oil may also be called "extra virgin". Raw oil is extracted by crushing and pressing copra. Various treatments are given to the raw oil to produce different products each with their own characteristics and hence applications. Refined coconut oil is also manufactured in the country for industrial uses. It is mainly used in the manufacture of confectionery items such as biscuits, chocolates, ice cream, pharmaceutical products and costly paints. It has various uses as cooking media, hair oil, body oil and industrial oil. Refined oil is virtually tasteless and odourless.

Coconut oil consists of predominantly triglycerides with 86.5 per cent saturated fatty acids, 5.8 per cent monounsaturated fatty acids and 1.8 per cent polyunsaturated fatty acids. Due to its typical fatty acid profile, the oil has a long shelf life compared to other oils because of its resistance to high temperature. Coconut oil is best stored in solid form, i.e. at temperatures lower than 76°F in order to extend shelf life. However, unlike most oils, coconut oil will not be damaged by warmer temperature. Among the most stable of all vegetable oils, coconut oil is slow to oxidize and thus resistant to rancidity.

The medium-chain fats in coconut oil are similar to fats in mother's milk and have similar nutritional effects. These health effects were recognized centuries ago in Ayurvedic medicine. The knowledge of the aborigines of Nicobar Islands and the tribal population of other parts of India on the medicinal application of coconut palm products is extensive. Even a transient account of ancient therapeutic applications of coconut palm products would be too extensive. Coconut oil nourishes the body and increases strength. The oil was and is also valued for its antimicrobial properties. The use of

the oil medicated with herbs is widespread among the people of India. Different preparations of coconut oil promote luxurious hair growth and protect the skin from bacterial, protozoal, and viral infections. For problems, such as lice, application of coconut oil medicated with the roots of coconut palm is known to be an effective treatment. Fresh lauric oil is wholesome to heart and relieves skin troubles. In the past four decades misinformation provided by certain politically biased agricultural groups and repeated in professional and lay press have led people to believe that all saturated fats are unhealthy. Little attention is focused on the fact that saturated fatty acids are not a single family of fats but comprises of three subgroups; short (C2-C6), medium (C8-C12) and long (C14-C24) chain fatty acids. The medium chain fats are found exclusively in lauric oils. Therefore it is important to understand the health benefits of medium chain saturated fats. It has been known for several years that subgroups existed for unsaturated fats. Little recognition is given even today to subgroups of saturated fats. Each fat subgroup has different metabolic, biological and pharmacological functions.

Apart from the application in edible area, due to its distinctive fatty acid profile, the oil has got wide range of applications in various fields like cooking media, personal care, skin care, home care, soaps, detergents etc. In this article, specifications of some of

the important chemicals derived from coconut oil have been discussed.

it should be identified that the oil in its native form will have the limited use in the field of lubrication due to

Table 1. Fatty acid profile of the refined coconut oil

Fatty acid	Chain length	Molecular formula	Molecular weight	Acid value	Melting point (°C)	Percentage (%)
Caproic acid	6:0	C ₆ H ₁₂ O ₂	166	483.62	-4	0.30
Caprylic acid	8:0	C ₈ H ₁₆ O ₂	144	389.98	16	0.26
Capric acid	10:0	C ₁₀ H ₂₀ O ₂	172	326.16	32	6.77
Lauric acid	12:0	C ₁₂ H ₂₄ O ₂	200	280.5	44	53.79
Myristic acid	14:0	C ₁₄ H ₂₈ O ₂	228	246.05	56	20
Palmitic acid	16:0	C ₁₆ H ₃₂ O ₂	256	219.14	63	8.12
Stearic acid	18:0	C ₁₈ H ₃₆ O ₂	284	197.53	69	2.43
Oleic acid	18:1	C ₁₈ H ₃₄ O ₂	282	198.93	18	6.78
Linoleic acid	18:2	C ₁₈ H ₃₂ O ₂	280	200.35	-6	1.24
Others	—	—	—	—	—	0.31
% Saturated	—	—	—	—	—	91.67
% Monounsaturated	—	—	—	—	—	6.78
% Diunsaturated	—	—	—	—	—	1.24
% Total Unsaturated	—	—	—	—	—	8.02

Applications of native coconut oil in various fields

Tribology: It is the science of friction, wear and lubrication. The properties mentioned in Table 2 help

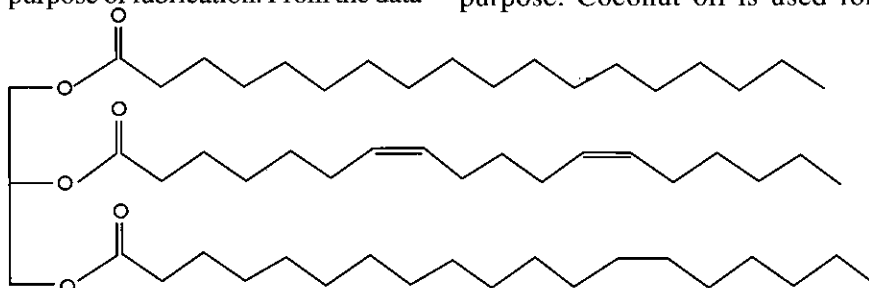
Table 2. Tribological properties of coconut oil

Characteristics	Value
Flash Point (°C)	263
Pour Point (°C)	15
Viscosity at 40°C	31.02
Viscosity at 100°C	9.8402
Viscosity Index	179.49
Copper Corrosion	1 (a)
Weld Load Load in Pan (Kg)	11
Actual (Kg X 15)	165
Newton (Kg X 15 X 9.8)	1,617

in understanding the possible use of coconut oil in its native form for the purpose of lubrication. From the data

its high pour point. However, the characteristics like viscosity, flash point, copper corrosion and weld load are good enough for some of the applications in lubrication field. In order to suit the oil for a particular application, the undesirable pour point (15°C) could be lowered by a suitable structural modification. The medium chain fatty acid may find use in synthesising newer class of lubricants of the desired range of properties.

Edible Oil: Coconut oil is commonly used in cooking, especially for frying, and it has a high smoke point temperature, which makes it good for this purpose. Coconut oil is used for



General structure of a triglyceride

making margarine, soap and cosmetics. Hydrogenated or partially-hydrogenated coconut oil is often used in non-dairy creamers and snack foods.

The requirement for specific gravity, refractive index, saponification value, iodine value and Polenske value are almost same for all grades. As the moisture content increases, there is increase in acid value, which reflects in lowering the flash point. (Table 3)

Table 3. IS: 542 – 1968 (Reaffirmed 1999) Specifications for coconut oil

Characteristics	Requirements for type						
	Expressed				Solvent extracted		
	Refined grade	Grade 1A (Raw)	Grade 1B (Raw)	Grade 2 (Raw)	Refined grade	Semi refined	Grade 1Raw
Moisture and insoluble impurities (% by Wt, Max.)	0.1	0.25	0.25	0.25	0.1	0.25	1.0
Colour (Lovibond Scale, 1" Cell, Y + 5R, Not deeper than)	2	4	11	30	2	10	30
Refractive index at 40°C	1.4480 to 1.4490						
Specific gravity at 30°C	0.915 to 0.920						
Saponification value (Min.)	250						
Iodine value (Wij's)	7.5 to 10	7.5 to 10	7.5 to 10	7.5 to 10	7.5 to 10	7.5 to 10	8 to 13
Acid value (Max)	0.5	2	6	8	0.5	1	10
Unsaponifiable matter (% by Wt, Max.)	0.5	0.8	0.8	0.8	0.5	0.8	1
Polenske value (Min)	13	13	13	—	13	—	—
Flash point (°C)	—	—	—	—	225	100	90

Use in cosmetics: Cosmetics are not the reaction products and composed of a blend of several ingredients to give the desired set of properties. Coconut oil is excellent as a skin moisturiser. A study showed that extra virgin coconut oil is effective and safe when used as a moisturiser, with absence of adverse reactions. In India and Sri Lanka, coconut oil is commonly used for styling hair, and cooling or soothing the head.

IS: 7123 – 1973 Specifications for Hair Oil

Three types of hair oils are used,

Type 1: Based on vegetable oil/ oils

Type 2: Based on mineral oil

Type 3: Based on a mixture of vegetable oil (s) – mineral oil emulsion

(**Vegetable Oils:** Castor oil, Coconut oil, Groundnut oil, Sesame oil, Mustard oil)

Oil along with colour and perfume should be packed in a well closed container.

Acid Value: Should not be more than 1.0

Peroxide Value: Should not be more than 7.5 milliequivalents/ 1000gm

Traditional fuel application:

Coconut oil was and is used in oil lamps since ancient times. Coconut oil had been tested for use as a feedstock for biodiesel (produced by transesterification of coconut oil using methanol and alkaline catalyst) to be used as a diesel engine fuel. In this manner it can be applied for power generation and transport using diesel engines. Raw coconut oil can be used as a fuel for generating electricity by remote communities that have an abundant supply of coconuts and milling capacity, provided diesel engines are adapted.

Specifications and utilization of cocochemicals derived from coconut oil

Glycerin: Glycerin is a byproduct of saponification reaction and fat splitting. The glycerin recovery is a significant factor in the economics of producing fatty acids and soaps from oils. The glycerin credit from biodiesel production has similarly increased the competi-

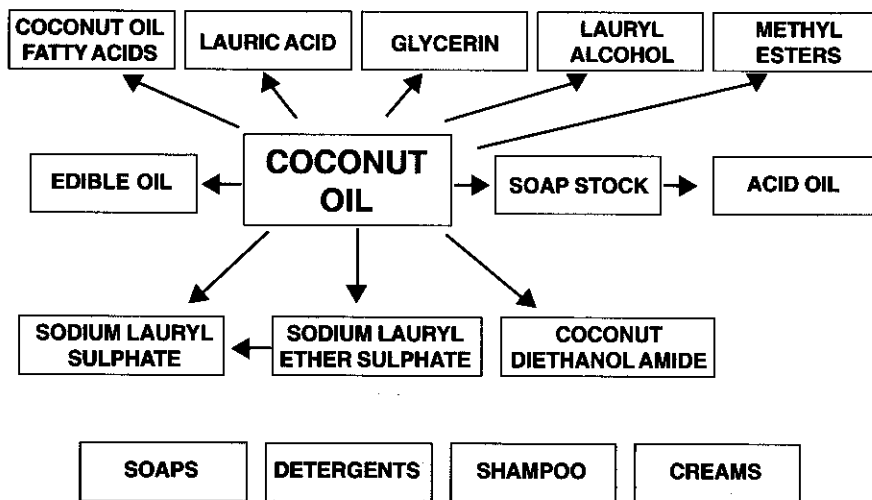
Table 4. IS: 11470 – 1985 (Reaffirmed 2006) Specifications for coconut oil for cosmetic industry

Characteristics	Requirements for	
	Type 1	Type 2
Moisture and insoluble impurities (% by Wt, Max.)	0.1	0.2
Colour (Lovibond Scale, 1" Cell, Y + 5R, Not deeper than)	2	10
Refractive index at 40°C	1.4480 to 1.449	
Specific gravity at 30°C	0.915 to 0.920	
Saponification value (Min.)	250	
Iodine value (Wij's)	7.5 to 10	
Acid value (Max)	0.5	2
Unsaponifiable matter (% by Wt, Max.)	0.5	0.8
Polenske value (Min)	13	—
Flash point (°C)	225	—
Test for rancidity	Shall be free from rancidity	

tiveness of that renewable fuel. Applications for glycerin include diverse products like drugs and

stringent as it gets accumulated in the body and is toxic to human beings.

the product depending on the quality of water used for saponification, fat splitting, the still in which the reaction, distillation and splitting is carried out.



Various uses of coconut oil and its derivatives

cosmetics, resins, polymers, and explosives. It has several commercial and industrial applications. The primary function of glycerin in many formulations is that of a humectant (a substance that retains moisture), as a carrier and emollient in cosmetics. It also acts as a solvent, sweetener, and preservative in food and beverages. Its properties as a plasticizer and biolubricant give it wide applicability for food processing machinery because of its nontoxic nature. It also finds application in the synthesis of alkyd resins to assure flexibility. Alkyd resins are used in products like paints and inks where brittleness is undesirable.

Based on the method of production, crude glycerin has different specifications as given in Table 5.

The ash content throws light on the metal content of the glycerin. Specifications for arsenic are

Table 5. IS: 1796 – 1961 Specifications for crude glycerin

Characteristics	Requirements	
	Soap Lye	Hydrolyser Grade
Glycerol (% by mass, Min)	80	88
Ash (% by mass, Max)	10	1.5
Non Volatile organic residue (% by mass, Max)	3	1.5
Arsenic as As (ppm, Max)	2	2
Total alkali (free and combined as Na ₂ O)	0.2	—

Specific gravity could be used as tool to know the purity of the product. The various metals come in

Cosmetics and toiletries: Humectant vehicle, and emollient in toothpaste, skin creams and lotions,

Table 6. IS: 1796 – 1961 Specifications for Refined glycerin

Characteristics	Requirements				
	Analytical reagent	Chemically pure	Industrial white	Technical	Dynamite grade
Glycerol (% by Weight, Min)	98	98	98	98	98.7
Specific gravity at 30°C (Min)	1.2552	1.2552	1.2552	1.2552	1.2571
Ash (% by Weight, Max)	0.01	0.01	0.01	0.05	0.025
Arsenic as As (ppm, Max)	1	2	—	—	—
Copper	To pass the test				
Iron as Fe (ppm, Max)	0.5	0.5	—	2	—
Lead as Pb (ppm, Max)	1	1	—	—	—
Chlorides as Cl (ppm, Max)	2	10	60	60	30
Sulphates as SO ₄ (ppm, Max)	10	10	—	—	—
Acidity or Alkalinity (Max)	Nil	Nil	0.01	0.01	0.01
Colour (Y + R) not deeper than	0.5	1	1	2.5	5
	(in 5.25" Cell)	(in 5.25" Cell)	(in 2" Cell)	(in 5.25" Cell)	(in 5.25" Cell)

shaving preparations, deodorants, and make up.

Tobacco: Keeps tobacco moist and soft to prevent breaking and crumbling during processing; ensures freshness in packaged cigarettes and other tobacco products.

Surface coatings: Used in the manufacture of alkyd resins, which are important component of surface coatings.

Paper and printing: Plasticizer, humectant, lubricant in the manufacture of paper, used with other ingredients in specialty treatments such as grease-proofing. Alkyd resins are important constituent of many printing inks.

Lubricants: Used due to its nontoxic character. It is used in lubricants for food and other machinery where product purity is essential.

Textiles: Conditioning agent used widely in lubricating, sizing, and softening yarn and fabric. Lubricates many kind of fibers in spinning, twist setting, knitting, and weaving operations.

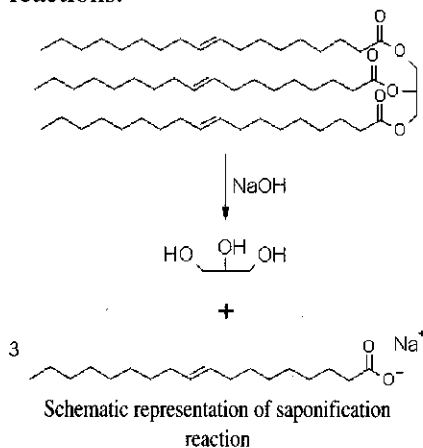
Rubber and plastics: Lubricant and plasticizer for plastics.

Urethane polymers: Fundamental chemical component of polyethers for urethane foams.

Electrical and electronics: Widely employed in manufacturing electrolytes for electrolytic condensers, which are used in radios and neon lights, and in processes for electro deposition and treatment of metals.

Nitration: Used to make nitroglycerin, which is the usual explosive in dynamite.

Coconut oil fatty acids: A range of fatty acids are derived from coconut oil from C8 to C18. The major fatty acids are lauric acid, myristic acid and palmitic acid. These fatty acids are produced by a process of saponification and acidulation and continuous high pressure fat splitting. Glycerin is obtained as a byproduct of these reactions.



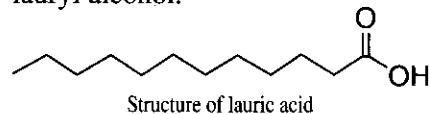
The fatty acids are further purified by fractional distillation to get the desired purity. The fatty acid profile of the distilled coconut fatty acids is summarized in Table 7.

Table 7. Fatty acid profile of distilled coconut fatty acid

Fatty acid	C ₈	C ₁₀	C ₁₂	C ₁₄	C ₁₆	C ₁₈	C _{18:1}	C _{18:2}
Percentage	1-2	3-4	50-56	14-18	8-10	1-2	8-11	1-2

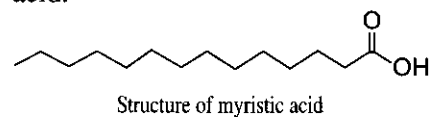
Out of the several fatty acids present in coconut oil, lauric acid is the most important one and is extensively used as intermediate for many reactions. The lauric acid is converted to lauryl alcohol by high pressure hydrogenation using a suitable catalyst and this product obtained is used in several formulations after derivatization such as soaps, shampoos, oral care products, personal care products, home care products, creams and lotions. However the BIS

specification is not available for lauryl alcohol.



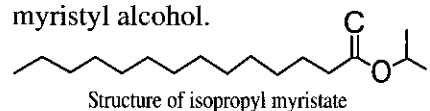
Acid value, saponification value, titre and iodine value reflects on the purity of the lauric acid. Unsaponifiable matter specifies the presence of hydrocarbons, pigments, fatty alcohols, sterols etc.

Myristic Acid: Even though important, there is no BIS specifications available for myristic acid.



However, the products derived from isopropyl myristate is included in the list of BIS specifications. This product is extensively used as one of the ingredient of cosmetic creams. Isopropyl myristate is an ester prepared by reacting myristic acid with excess of isopropyl alcohol using acidic catalyst. The myristic

acid is converted to myristyl alcohol by high pressure hydrogenation using a suitable catalyst and the product finds use in preparation of synthetic wax, formulation of detergents etc. However the BIS specification is not available for myristyl alcohol.



Acid value of the final product defines the completion of esterification reaction. Saponi-

Table 8. IS: 10931 – 1984 (Reaffirmed 2006) Specifications for lauric acid

Characteristics	Requirements for		
	Grade 1	Grade 2	Grade 3
Lauric acid (% by Mass, Min.)	99	90	70
Moisture (% by Mass, Max.)	0.1	0.1	0.1
Saponification value	279-281	276-284	272-290
Acid value shall not differ from SV by more than	4	4	4
Iodine value (Wij's)	0.1	0.5	1.0
Mineral acidity	Nil	Nil	Nil
Ash (% by mass, Max)	0.01	0.01	0.02
Unsaponifiable matter (% by Mass Max)	0.1	0.1	0.2
Titre (°C)	43-44	39-44	35-43
Colour (51/4" Cell Y + 5R) Max	2	5	10

fication value, acid value, iodine value and titre of separated fatty acid reflect on the purity of the myristic acid taken for the reaction. Residue on ignition tells about the metal contaminants.

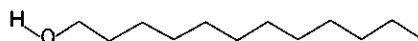
material for the production of fatty sulfate salts and alcohol ethoxylates for foaming and cleaning purposes in the field of detergent industry. Chemical reactions of primary alcohols include esterifications,

Table 9. IS: 1356 – 1983 Isopropyl Myristate

Characteristics	Requirements
Acid Value (Max)	1.0
Titre of separated fatty acids (°C)	47 to 53
Saponification Value	190 to 220
Iodine value (Max)	1.0
Arsenic (ppm, Max)	2
Heavy Metals (ppm, Max)	30
Specific gravity at 20°C	0.847 to 0.853
Residue on ignition (% by Mass, Max)	0.02

Fatty alcohols: These are derived from natural oils and fats and are straight chain, high molecular weight primary alcohols. They include lauryl (C12), myristyl (C14), cetyl (C16), stearyl (C18), oleyl (C18, unsaturated) and so on. Fatty alcohols are emulsifiers and emollients to make skin smoother and prevent moisture loss. Identical fatty esters are used to improve rub-out of formulas and to control viscosity and dispersion characteristics in cosmetics, personal care products and pharmaceutical ingredients. As chemical intermediates, the primary use of fatty alcohols is as raw

ethoxylation, sulfation, oxidation and many other reactions.



Structure of lauryl alcohol

Soap Stock: It is a byproduct obtained in the refining step of coconut oil. The separate specification for coconut oil soap stock is not available. Soap stock is complex mixture of sodium salt of

fatty acid, moisture, colour bodies, phospholipids, excess of alkali and neutral oil or triglyceride. It is a moist or wet, sticky and dark coloured mass. The general specification for soap stock is given in Table 10. The advantage is that this byproduct of edible oil refining is less expensive than edible grade refined oils. The most effective method involved is complete saponification of the soapstock, followed by acidulation using methods similar to those, which are presently employed in industry. This result in acid oil formation with a higher free fatty acid content, ie. more than 50 per cent. These fatty acids are efficiently converted to methyl esters by acid-catalyzed esterification, resulting in a product that meet the accepted US specifications for biodiesel.

Total fatty matter represents the amount of fatty acids present. The amount of fatty matter is quite less due to the presence of many components. Oxidized fatty acids give the idea about the off odour associated with the product.

Acid oil: Soap stock is an organic mass having sufficient quantity of moisture and hence is prone for the microbial and oxidative degradation. Therefore, it is not stored as such but converted to acid oil. Soap stock is boiled with excess of water and is acidified to yield the corresponding fatty acids. Acid oil is a mixture of neutral oil and substantial quantity

Table 10. IS: 12031 – 1986 (Reaffirmed 1998) specifications for soap stock

Characteristics	Requirements
Total fatty matter (% by Mass, Min.)	20
pH Min	7.0
Unsaponifiable matter on TFM (% by Mass Max)	5.0
Oxidized fatty acids (% by Mass on TFM, Max)	5.0

of free fatty acids, hence the name acid oil. This product is generally dark coloured. Now a days efforts are being made to produce the

and cleaning properties. It promotes better, more efficient combustion and less engine vibration because of its higher cetane number and

inherent oxygen content. It also boosts engine power and acceleration improves fuel economy by as much as 20 per cent, which means you get more mileage and big savings per liter. Separate specifications for cocobiodiesel are not available. The specifications of biodiesel in general are summarized in Table 12.

Coco-Biodiesel results in better combustion, less pollution, and more engine power; the engines run smoothly and with longer

Table 11. IS: 12029 – 1986 Specifications for acid oil

Characteristics	Requirements
Total fatty matter (% by Mass, Min.)	95
Moisture and volatile matter content (% by Mass, Max.)	4.0
Free fatty acid (% by Mass Min)	50
Free mineral acid (as H ₂ SO ₄ , % by Mass Max)	0.02
Unsaponifiable matter on TFM (% by Mass Max)	5.0
Oxidized fatty acids (% by Mass on TFM, Max)	5.0
Iron (ppm Max)	500
Ash (% by mass, Max)	0.25

biodiesel from this cheaper source of fatty feed stock. Since the separate specification for the acid oil derived from coconut oil is not available a common specification applicable is given in Table 11.

The acid oil contains good amount of fatty matter as compared to soap stock and saves the transportation cost. The specifications for the presence of mineral acidity are stringent as it leads to increase in acid value. Even the traces of mineral acidity can have the profound effect on the final acid value of the acid oil. Specs for iron are specified as it is a pro-oxidant and catalyses the oxidation reaction, while oxidized matter is responsible for off odour of the product.

Coconut oil methyl esters: It is referred to as cocobiodiesel. The Philippines has launched the use of biodiesel, particularly, coconut methyl ester or CME, which is derived from coconut oil. Compared with other forms of biodiesels, the medium carbon chain of Coco-Biodiesel offers excellent lubricity, solvency and detergency. Coco-biodiesel cuts the maintenance cost because of its superior lubricating

Table 12. Indian bio-diesel specifications from Society of Indian Automobile Manufacturers

Characteristics	Requirement	Method of Test, ref to	
		Other methods	[P:] of IS 1448
(1)	(2)	(3)	(4)
Density at 15°C, kg/m ³	860-900	ISO 3675	P:16/
		ISO 12185	P:32
		ASTM	
Kinematic viscosity at 40°C, cSt	2.5-6.0	ISO 3104	P:25
Flash point (PMCC) °C, min	120	P:21	
Sulphur, mg/kg max.	50.0	ASTM D 5453	P:83
Carbon residue (Ramsbottom) *, % by mass, max	0.05	ASTM D 4530/ISO 10370	-
Sulfated ash, % by mass, max	0.02	ISO 6245	P:4
Water content, mg/kg, max	500	ASTM D 2709	P:40
		ISO 3733	
		ISO 6296	
Total contamination, mg/kg, max	24	EN 12662	-
Cu corrosion, 3 hrs at 50°C, max	1	ISO 2160	P:15
Cetane No., min	51	ISO 5156	P:9
Acid value, mg KOH/g, max	0.50	-	P:1 / Sec 1
Methanol @, % by mass, max	0.20	EN 14110	-
Ethanol, @@ % by mass, max	0.20	-	-
Ester content, % by mass, min	96.5	EN 14103	-
Free glycerol, % by mass, max	0.02	ASTM D 6584	-
Total glycerol, % by mass, max	0.25	ASTM D 6584	-
Phosphorous, mg/kg, max	10.0	ASTMD 4951	-
Sodium & Potassium, mg/kg, max	To report	EN 14108 &	-
	EN 14109	-	-
Calcium and Magnesium, mg/kg, max	To report	**	-
Iodine value	To report	EN 14104	-
Oxidation stability, at 110°C hrs, min	6	EN 14112	-

*Carbon residue shall be run on 100% sample.

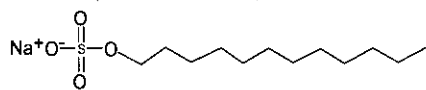
** European method is under development

@ Applicable for Fatty Acid Methyl Ester

@@ Applicable for Fatty Acid Ethyl Ester

maintenance intervals. It is renewable and biodegradable, being plant-based, lowers emission of sulfur oxide, which is the main contributor to smog. It also significantly reduces serious air pollutants such as black smoke and air toxics that cause lung cancer, pulmonary tuberculosis, pneumonia, bronchitis and heart attack. It could establish a sustainable alternative domestic market for coconut oil and as a result, will stabilize the domestic coconut production, resulting in more income from copra, enhancing farm-based reintegration of opportunities.

Sodium lauryl sulphate: It is prepared by treating lauryl alcohol with sulfuric acid or oleum or sulfur trioxide and subsequently neutralized by sodium hydroxide. It is commonly referred to as SLS or Sodium dodecyl sulfate (SDS or NaDS). The chemical



Structure of sodium lauryl sulphate

formula is $\text{CH}_3(\text{CH}_2)_{11}\text{OSO}_3\text{Na}$. It is an anionic surfactant, which is used as a foaming agent (to clean and make bubbles) in a large variety of used products. These include shampoos, soaps, face and body washes, toothpaste, laundry detergents and industrial cleansing chemicals such as engine degreasers. There are many derivatives of SLS that can be found in commercial preparations, including sodium laureth sulphate, sodium laureth-3 sulphate, and di ethanol amine (DEA) or tri ethanol amine (TEA) and sodium lauryl sulphate. Although these derivatives vary slightly in mildness, the general action and effects are essentially similar. A major concern about SLS is its effect,

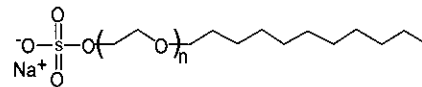
Table 13. IS: 3986 – 1988 (Reaffirmed 2005, Third Revision) Specifications for sodium lauryl sulphate

Characteristics	Requirements for		
	Type 1	Type 2	Type 3
Sodium lauryl sulphate (% by Mass, Min.)	94	85	30
Unsulphated fatty alcohols (% by Mass, Max.)	1	2.5	1.1
Arsenic as (As_2O_3) (ppm Max)	2	2	1
Heavy metals (as Pb) (ppm Max)	20	20	20
Sodium chloride (% by Mass, Max.)	1	1.5	1
Sodium sulphate (% by Mass, Max.)	2	6	4
Alkalinity	To Pass the Test		
pH (1% solution)	7.5-10.5	7.5-10.5	7.5-11

when used in combination with other chemicals or ingredients commonly found in personal care products. There are several other surfactants with similar names to SLS – in particular ammonium lauryl sulphate and ammonium laureth sulphate. Although these sound very similar, their molecular structure is significantly different and they do not have the same potential to irritate the skin. Also, because their molecules are larger than those of SLS, they are not able to pass through the skin and therefore cannot be absorbed into the body in the same way. Because of these differences, ammonium lauryl and laureth sulphates are considered to be milder and safer alternatives to SLS. Table 13 summarises the specifications for sodium lauryl sulphate.

Depending on the requirement of end application and type, the specifications of sodium lauryl sulphate are available for 30 per cent to 94 per cent. Unsulphated fatty alcohol gives idea about the completion of reaction. Alkalinity tells about the presence of excess alkali.

Sodium lauryl ether sulphate: Lauryl alcohol is ethxylated and the ethoxylated mass is reacted with



Structure of sodium lauryl ether sulphate

sulfuric acid and the product obtained is neutralized with sodium hydroxide. It is used in many personal care products like soaps, liquid soaps and shampoos, bubble

Table 14. IS: 11487 – 1985 (Reaffirmed 2006) Specifications for sodium lauryl ether sulphate (30% solution)

Characteristics	Requirements
Active detergent (% by Mass, Min.)	27
Non detergent organic matter (% by Mass, Max.)	2.5
Sodium chloride and sodium sulphate (% by Mass Max)	3.5
Cloud point ($^{\circ}\text{C}$)	Less than 0
Viscosity (cP at 27°C)	1,500 to 5,000
Heavy metals (as Pb) (ppm, Max)	20
Arsenic (As_2O_3) (ppm Max)	2
pH (5% aqueous solution)	6 to 8
Iron (as Fe) (ppm Max)	20
Formalin (% by Mass Max)	0.04
1,4 Dioxane on 100% basis, (ppm Max)	100

baths, bath and shower gels, toothpaste etc. due to its effective foaming property. Its chemical formula is $\text{CH}_3(\text{CH}_2)_{10}\text{CH}_2(\text{OCH}_2\text{CH}_2)_n\text{OSO}_3\text{Na}$. Sometimes the number represented by "n" is specified in the name, for example laureth-2 sulfate. The commercial product is heterogeneous, both in the length of the alkyl chain (12 being the mode of the number of carbon atoms), and in the number of ethoxyl groups, where n is the mean. n=3 is common in commercial products.

Non detergent organic matter is the ethoxylated mass. Cloud point gives the temperature at which the surfactant comes out of solution. Formalin (mixture of formic acid, methanol and water in a ratio of 37:13:50) is used as a preservative. Dioxane is a toxic compound that gets generated during the ethoxylation.

Ammonium lauryl sulfate (ALS): The chemical formula is $\text{CH}_3(\text{CH}_2)_{10}\text{CH}_2\text{OSO}_3\text{NH}_4$, which is an anionic surfactant used in cosmetic formulations, with some shampoos containing up to 30 per cent ALS. It is most widely used in the USA. In Europe sodium laureth sulfate is used instead because ammonium lauryl sulfate gives off ammonia odor in alkaline pH. The lauryl sulfates are used because they are very high foamers but not an effective cleaner, thus will not "de-oil" as would the more common Dodecyl benzene sulfonates found in most US hand dishwashing compounds. Ammonium lauryl sulfate, like any other surfactant, makes a good base for cleansers as it disrupts the hydrogen bonding in water. Hydrogen bonding is the cause of "water tension". In solution, the lauryl sulfate molecules ionize,

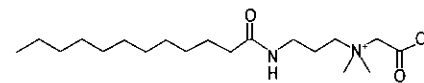
meaning that the ammonium or sodium separates from the rest of the molecule as a +1 ion. The rest of the molecule aligns itself with others like it and forms what is known as a micelle. The molecules align themselves in a sphere, with the polar heads (the sulfate) on the surface of the sphere and the polar hydrophobic tails pointing inwards towards the center. The water molecules around the micelle arrange themselves around the polar heads, but this disrupts their hydrogen bonding with the water surrounding them. The overall effect of having these micelles in an aqueous (water) environment is that the water becomes more able to penetrate things like cloth fibers or hair, and also becomes more readily available to solvate anything coming off the before mentioned substance.

Coconut diethanol amide: This product finds application as foam booster and is synthesized by reaction between coconut fatty acids and diethanol amine.

Free acidity tells about the extent of reaction. Total fatty acids give the total fatty matter present. Acid value of the separated fatty acids reflects

on the authenticity of the raw material.

Cocamidopropyl betaine: It is commonly referred as CAPB (N-(carboxy methyl)-N,N-Dimethyl-3-[(1-Oxococonut) amino]-1-Propanaminium Hydroxide). Cocamidopropyl betaine is a derivate of cocamide and betaine. It is an amphoteric or zwitter ionic surfactant with a quaternary ammonium cation in its molecule that can act as an acid or a base. It is a viscous pale yellow transparent



Structure of cocoamido propyl betain

liquid and is used as a surfactant in personal care products like shampoos and hand soaps. In cosmetic formulations, it is used as an emulsifying agent, thickener and to reduce irritation, which purely ionic surfactants would cause. It also serves as an antistatic agent in hair conditioners. It does not irritate the skin or mucous membranes. It has antibiotic effects, and is used in personal sanitary products. It has anti-static properties, making it a conditioning agent in shampoos.

Table 15. IS: 7101 - 1994 (Second Revision) Specifications for coconut diethanol amide

Characteristics	Requirements	
	Grade 1	Grade 2
Free fatty acid as Lauric Acid (% by Mass, Max.)	0.5	1
Direct titratable amine (as diethanolamine) % Mass, Min.)	9	18
Combined amine (as diethanolamine) % Mass, Min.)	31	20
Sulphated ash (% by Mass, Max.)	1	1
Moisture (% by Mass, Max.)	1	1
Total fatty acids (% by Mass, Min.)	62	43
Acid value of separated fatty acids	255 to 280	255 to 280
pH (10% solution)	9 to 10.5	—
Heavy metals (as Pb) (ppm Max)	20	20
Arsenic (as As) (ppm Max)	2	2

It is compatible with other cationic, anionic, and nonionic surfactants. However, the BIS specifications are not available for coco amido propyl betaine.

General applications of the cocochemicals in various industrial segments

Personal care: It is used in the form of fatty alcohol, fatty alcohol ethoxylates, quaternary ammonium salts, amine oxides, fatty amines and esters. These chemicals perform various roles such as conditioners, thickeners, superfatting agents, emollients, viscosity builders, gelling agents, solubilisers, dispersants and emulsifiers. These products find use in several formulations like creams, shampoos, hair products, skin products, shaving products, bath oils, lotions, perfumed products, hair products, medicated cosmetics, lipsticks, sunscreens etc.

Detergents: Fatty alcohol sulfates and alcohol ether sulfates (alcohol ethoxysulphates), alcohol ethoxylates, quaternary ammonium salts, fatty amines and amine oxide are used to perform functions like foam controller, emollient, opacifier, surfactants, softeners, wetting agents, dispersants, emulsifiers, softeners, foam stabilizes, etc. These chemicals are used in formulations like laundry powders, light and heavy duty dishwashing, wool washing, liquid detergents, fabric softeners etc.

Surface cleaners: Cocochemicals in the form of alcohol sulfates, ether sulfates (ethoxysulfates), fatty amines, amine oxide, quaternary ammonium salts etc. are used for

various roles as foam controllers, wetting agents, dispersants, surfactants and germicidal disinfectants. These are used in the formulations such as floor, toilet, metal, bottle and scouring cleaners.

General industrial applications: Alcohol / alcohol ethoxylates / quaternary ammonium salts are used to perform particular function in several industrial applications given below.

Textile chemicals: Used as fabric softners.

Leather industry: Foam controller and leveling agent.

Paper industry: For control of surface tension, de-foaming and de-inking applications.

Polymers: It is used as lubricant additives, polymerization auxiliaries, plasticizers, foam stabilizers, etc.

Metal working oils: It is used as rolling oils, hydraulic oils and anti-corrosion agents.

Water treatment: As a bacteriostat.

Foods and pharmaceuticals: Deodorant, depilatories, ointments and emulsifiers.

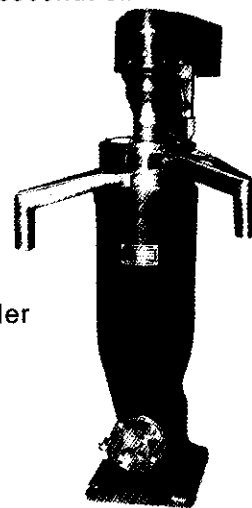
Summary

Coconut oil is primarily used for edible purpose and as a hair oil. It is an important source of intermediates like fatty acids, glycerol and fatty alcohols, which are used for the manufacture of wide range of chemicals such as surfactants, emulsifiers, foam boosters etc. These intermediates are used in the formulation of several finished products like soaps, detergents and shampoos. Glycerol is used in lot of cosmetics formulations. Palm kernel oil also has a similar fatty acid profile. It could be used for the manufacture of all the cocobased chemicals. However the cocobased products are preferred due to their characteristic odour and mind set of the people.

Tubular Bowl Centrifuge for purification of coconut oil

Plant and Equipment
for the production
of **Virgin coconut oil**

Vibrating Screen for
desicated coconut powder



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